

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims:

1. (Currently Amended) A parallel computing method for executing calculation of the Hartree-Fock method in a molecular orbital method, comprising the steps of:

using a computer cluster made up of a plurality of computers and a communication device coupled to said plurality of computers, each of said plurality of computers having a memory capacity which is insufficient to store whole matrices used in Hartree-Fock calculation;

dividing a density matrix into multiple density submatrixes and distributing the multiple density submatrixes to the multiple computers and storing therein; and

executing calculation processes on the density submatrixes in each of the computers while sequentially transferring the multiple density submatrixes between the multiple computers via said communication device.

2. (Currently Amended) The method according to Claim 1, wherein a duplication of the density matrix is used, and the density matrix and the duplication are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers via said communication device to thereby reduce calculation of integrals.

3. (Currently Amended) The method according to Claim 1, wherein the density matrix and duplications of the density matrix, four in total, are used, and the density matrix and the duplications are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers via said communication device, to thereby reduce calculation of integrals, by using symmetry of $(rs|u) \leftrightarrow (tu|rs)$ in two-electron integration.

4. (Original) The method according to Claim 1, further comprising the step of:
partially executing two-electron integration in each of the computers and updating the stored density submatrixes based on the result of the two-electron integration.

5. (Currently Amended) The method according to Claim 4, wherein a duplication of the density matrix is used, and the density matrix and the duplication are individually divided into density submatrices, causing the density submatrices to transfer between the computers via said communication device, to thereby reduce calculation of integrals.

6. (Currently Amended) The method according to Claim 4, wherein the density matrix and duplications of the density matrix, four in total, are used, and the density matrix and the duplications are individually divided into density submatrices, causing the density submatrices to transfer between the computers via said communication device, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \leftrightarrow (tu|rs)$ in two-electron integration.

7. (Currently Amended) A parallel computing system for executing calculation of the Hartree-Fock method in a molecular orbital method, comprising:

a computer cluster made up of a plurality of computers and a communication device coupled to said plurality of computers,

each of the computers comprising a matrix storage for storing density submatrices which are divided from a density matrix; a transfer controller for performing transmission and reception of the density submatrices with respect to the other computers in the computer cluster; and a calculation processor for performing a calculation on the density submatrix stored in the matrix storage,

wherein said each matrix storage has a memory capacity which is insufficient to store whole matrices used in Hartree-Fock calculation, initial values of the density submatrices are supplied to the matrix stages of the respective computers, calculation processes on the density submatrices are executed in each of the computers while the multiple density submatrices are being sequentially transferred between the multiple computers via said communication device, and resultant Fock matrix can be obtained by combining resultant Fock submatrices stored in said matrix storages of said plurality of computers.

8. (Currently Amended) The system according to Claim 7, wherein said storage stores two groups of the density submatrices which are obtained by individually dividing the

density matrix and a duplication of the density matrix ~~are individually divided into density submatrixes, causing the two groups of the density submatrixes to transfer~~ are transferred between the computers via said communication device, to thereby reduce calculation of integrals.

9. (Currently Amended) The system according to Claim 7, wherein said storage stores four groups of the density submatrixes which are obtained by individually dividing the density matrix and duplications of the density matrix, four in total, are individually divided into density submatrixes, causing and the four groups of the density submatrixes to transfer are transferred between the computers via said communication device, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \leftrightarrow (tu|rs)$ in two-electron integration.

10. (Original) The system according to Claim 7, wherein the calculation processor partially executes two-electron integration and the density submatrix in the matrix storage is updated based on the result of two-electron integration.

11. (Currently Amended) The system according to Claim 10, wherein said storage stores two groups of the density submatrixes which are obtained by individually dividing the density matrix and a duplication of the density matrix ~~are individually divided into density submatrixes, causing the two groups of the density submatrixes to transfer~~ are transferred between the computers via said communication device, to thereby reduce calculation of integrals.

12. (Currently Amended) The system according to Claim 10, wherein said storage stores four groups of the density submatrixes which are obtained by individually dividing the density matrix and duplications of the density matrix, four in total, are individually divided into density submatrixes, causing and the four groups of the density submatrixes to transfer are transferred between the computers via said communication device, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \leftrightarrow (tu|rs)$ in two-electron integration.

13. (Currently Amended) A computer readable medium storing a computer program causing a computer at each node in a computer cluster constituted by a plurality of nodes and a communication device coupled to said plurality of nodes, to function as:

a matrix storage for storing density submatrixes which are divided from a density matrix; a transfer controller for performing transmission and reception of the density submatrixes with respect to the other nodes in the computer cluster; and a calculation processor for performing a calculation on the density submatrix stored in the matrix storage,

whereby said each matrix storage has a memory capacity which is insufficient to store whole matrices used in Hartree-Fock calculation, initial values of the density submatrixes are supplied to the matrix stages of the respective nodes, calculation processes on the density submatrixes are executed at each of the nodes while the multiple density submatrixes are being sequentially transferred between the multiple nodes via said communication device, and resultant Fock matrix can be obtained by combining resultant Fock submatrixes stored in said matrix storages of said plurality of nodes.

14. (Canceled).

15. (New) The method according to Claim 1, further comprising:

computing, using the multiple density submatrixes being transferred between said plurality of computers, precise simulations of structures and physical properties of molecules, and chemical bonds, molecular orbitals and electron states in molecules,

wherein no high-performance computers are included in said plurality of computers making up the computer cluster.

16. (New) The method according to Claim 1, wherein the executing step is performed by each of said plurality of computers making up the computer cluster.

17. (New) The system according to Claim 7, wherein the multiple density submatrixes are transferred between said plurality of computers, so as to obtain precise simulations of structures and physical properties of molecules, and chemical bonds, molecular orbitals and electron states in molecules, and

wherein no high-performance computers are included in said plurality of computers making up the computer cluster.

18. (New) The computer readable storage medium according to Claim 13, wherein the multiple density submatrixes are transferred between said plurality of computers, so as to obtain precise simulations of structures and physical properties of molecules, and chemical bonds, molecular orbitals and electron states in molecules, and

wherein no high-performance computers are included in said plurality of computers making up the computer cluster.

19. (New) A parallel computing method for executing calculation of the Hartree-Fock method in a molecular orbital method, comprising the steps of:

using a computer cluster made up of a plurality of computers;

dividing a density matrix into multiple density submatrixes and distributing the multiple density submatrixes to the multiple computers making up the computer cluster and storing therein;

executing, in each of the multiple computers of the computer cluster, calculation processes on the density submatrixes while sequentially transferring the multiple density submatrixes between the multiple computers; and

computing, using the multiple density submatrixes being transferred between the multiple computers, precise simulations of structures and physical properties of molecules, and chemical bonds, molecular orbitals and electron states in molecules,

wherein no high-performance computers are included in the multiple computers making up the computer cluster.